

Cyclosarin
329-99-7 | DTXSID00861875

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 5.79

Global applicability domain: Inside

Local applicability domain index: 9.63e-01

Confidence level: 8.38e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Chloronaphthalene</div> <div>Measured: 5.80</div> <div>Predicted: 5.80</div>	<div>Image not found</div> <div>2-Chloronaphthalene</div> <div>Measured: 5.80</div> <div>Predicted: 5.80</div>	<div>Image not found</div> <div>1,2,4,5-Tetrachlorobenzene</div> <div>Measured: 5.63</div> <div>Predicted: 5.67</div>
<div>Image not found</div> <div>Biphenyl</div> <div>Measured: 6.15</div> <div>Predicted: 5.83</div>	<div>Image not found</div> <div>1,2,3,5-Tetrachlorobenzene</div> <div>Measured: 5.55</div> <div>Predicted: 5.67</div>	